

chain nodes :

1 3 4 5 6 7 8 17 21 22 23 25 26 27 28 29 30 31 32 33 34 35 36 37
 38 39 40 41 42 43 44 45 46 47 48 50 51 52 53 68 69 71 72 73 74 78
 79 80 81 82 83 87

ring nodes :

9 10 11 12 13 14 62 63 64 65 66 67

ring/chain nodes :

2 15

chain bonds :

1-3 1-4 2-78 3-87 5-21 6-7 6-8 6-15 22-71 22-23 25-26 26-27 28-29 28-30
 31-32 32-33 34-35 34-36 37-39 38-39 39-40 41-42 42-43 42-44 45-47 46-47 47-48
 50-52 51-52 52-53 62-63 62-66 63-64 63-68 64-65 65-66 66-67 68-69 72-73 72-74 79-80 79-81 80-82 81-83

ring/chain bonds :

1-2

ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14 62-63 62-66 63-64 64-65 65-66

exact/norm bonds :

1-2 1-3 1-4 2-78 3-87 5-21 6-7 6-8 6-15 22-71 22-23 25-26 26-27 28-29 28-30
 31-32 32-33 34-35 34-36 37-39 38-39 39-40 41-42 42-43 42-44 45-47 46-47 47-48
 50-52 51-52 52-53 62-63 62-66 63-64 63-68 64-65 65-66 66-67 68-69 72-73 72-74
 79-80 79-81 80-82 81-83

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14

G1: [*1], [*2], [*3]

G2: O, S

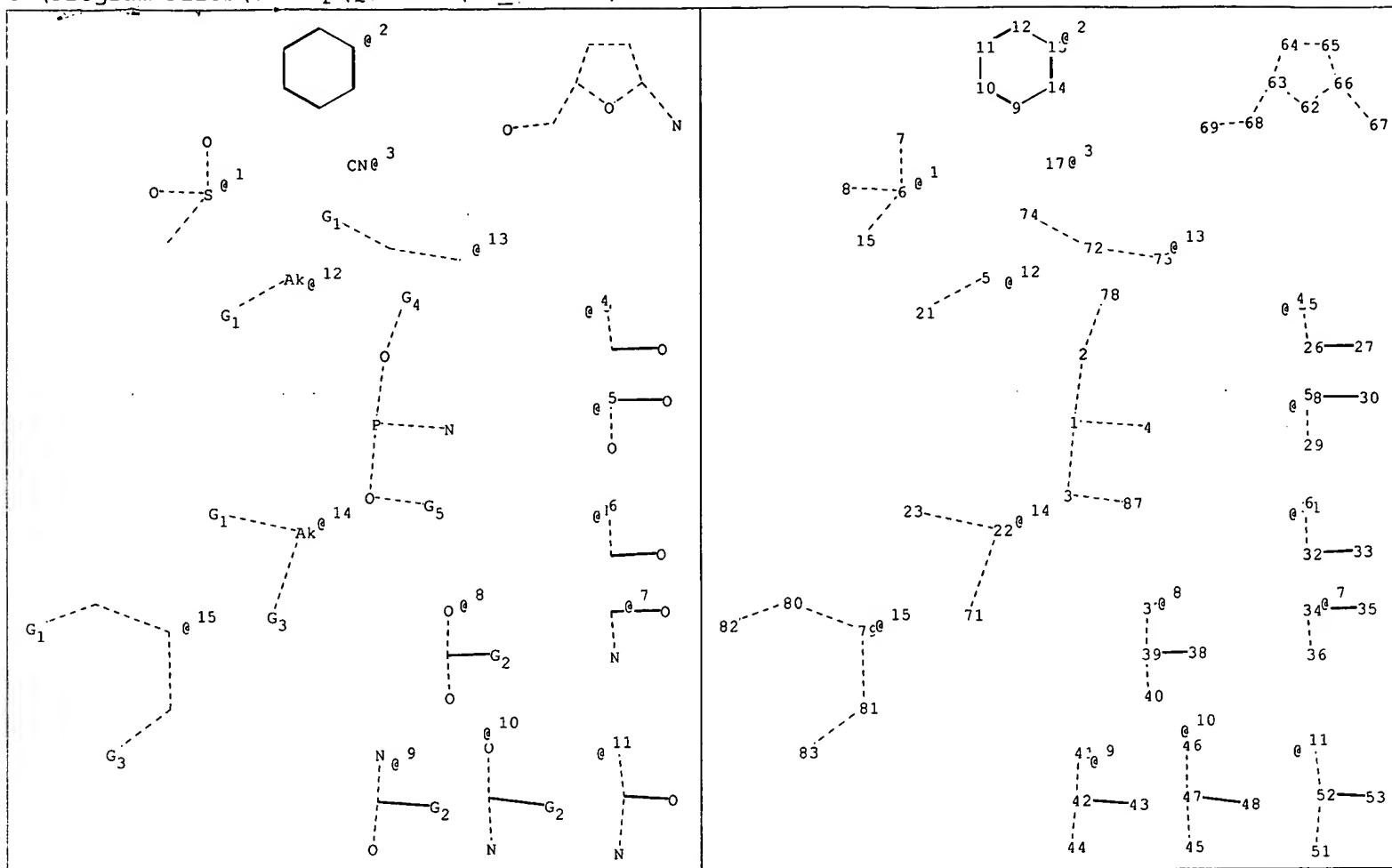
$$G_3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]$$

G4: [*12], [*13]

G5: [*14], [*15]

Match level :

1:CLASS	2:CLASS	3:CLASS	4:CLASS	5:CLASS	6:CLASS	7:CLASS	8:CLASS	9:Atom	10:Atom
11:Atom	12:Atom	13:Atom	14:Atom	15:CLASS	17:CLASS	21:CLASS	22:CLASS	23:CLASS	
25:CLASS	26:CLASS	27:CLASS	28:CLASS	29:CLASS	30:CLASS	31:CLASS	32:CLASS	33:CLASS	
34:CLASS	35:CLASS	36:CLASS	37:CLASS	38:CLASS	39:CLASS	40:CLASS	41:CLASS	42:CLASS	
43:CLASS	44:CLASS	45:CLASS	46:CLASS	47:CLASS	48:CLASS	50:CLASS	51:CLASS	52:CLASS	
53:CLASS	62:Atom	63:Atom	64:Atom	65:Atom	66:Atom	67:Atom	68:CLASS	69:CLASS	
71:CLASS	72:CLASS	73:CLASS	74:CLASS	78:CLASS	79:CLASS	80:CLASS	81:CLASS	82:CLASS	
83:CLASS	87:CLASS								



chain nodes :

1 2 3 4 5 6 7 8 17 21 22 23 25 26 27 28 29 30 31 32 33 34 35 36
 37 38 39 40 41 42 43 44 45 46 47 48 50 51 52 53 68 69 71 72 73 74
 78 79 80 81 82 83 87

ring nodes :

9 10 11 12 13 14 62 63 64 65 66 67

ring/chain nodes :

15

chain bonds :

1-2 1-3 1-4 2-78 3-87 5-21 6-7 6-8 6-15 22-71 22-23 25-26 26-27 28-29 28-30
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ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14 62-63 62-66 63-64 64-65 65-66

exact/norm bonds :

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normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14

G1: [*1], [*2], [*3]

G2: O, S

G3: [*4], [*5], [*6], [*7], [*8], [*9], [*10], [*11]

G4: [*12], [*13]

G5: [*14], [*15]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:CLASS 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 17:CLASS 21:CLASS 22:CLASS 23:CLASS
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:CLASS 39:CLASS 40:Atom 41:Atom 42:CLASS 43:CLASS
44:Atom 45:Atom 46:Atom 47:CLASS 48:CLASS 50:CLASS 51:Atom 52:Atom 53:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:CLASS 69:Atom 71:CLASS
72:CLASS 73:CLASS 74:CLASS 78:CLASS 79:CLASS 80:CLASS 81:CLASS 82:CLASS 83:CLASS
87:CLASS